Numerical Integration

1. Quadrature Rules
   - formulas for numerical integration
   - deriving quadrature rules

2. Composite Quadrature Rules
   - the composite trapezoidal rule
   - a Julia function

3. Newton-Cotes Formulas
   - integrate the interpolating polynomial

MCS 471 Lecture 25
Numerical Analysis
Jan Verschelde, 20 October 2021

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quadrature rules

Given a function $f(x)$ over an interval $[a, b]$,
our problem is to approximate the definite integral of f over $[a, b]$,
by a weighted sum of function values:

$$\int_a^b f(x)dx \approx w_1 f(x_1) + w_2 f(x_2) + \cdots + w_n f(x_n).$$

The *quadrature rule* is defined by

- interpolation points $x_i \in [a, b]$, $x_1 < x_2 < \cdots < x_n$; and
- weights w_i to multiply the function values with.

the midpoint and trapezoidal rule

The midpoint rule is defined by

$$\int_a^b f(x)dx \approx (b-a)f\left(\frac{a+b}{2}\right).$$

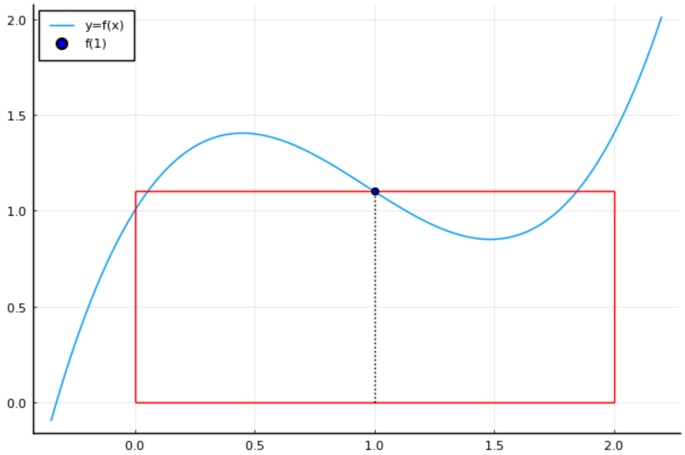
The area under $y = f(x)$ is approximated
by the area of the rectangle with base $b-a$ and height $f((a+b)/2)$.

The trapezoidal rule is defined by

$$\int_a^b f(x)dx \approx \frac{b-a}{2}\left(f(a)+f(b)\right).$$

The area under $y = f(x)$ is approximated
by the area of the trapezoid with base $b-a$ and heights $f(a)$ and $f(b)$.

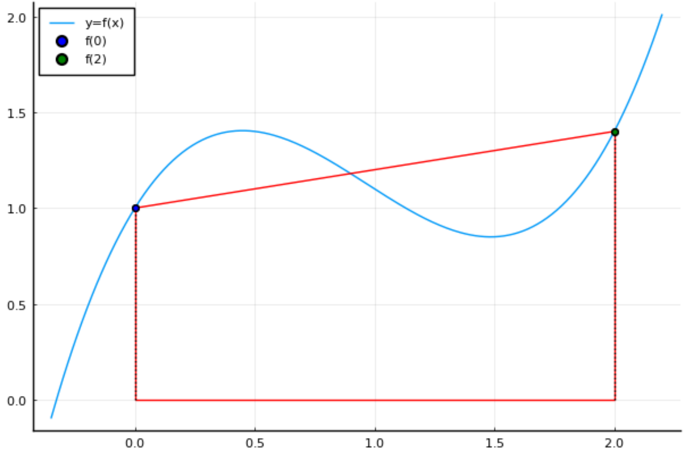
the midpoint rule



$\int_0^2 f(x)dx$, the area under the blue curve, for $x \in [0,2]$,

is approximated by $2\,f(1)$, the area of the red rectangle.

the trapezoidal rule



$\displaystyle\int_0^2 f(x)dx$, the area under the blue curve, for $x \in [0,2]$,

is approximated by $\frac{2-0}{2}(f(2) - f(0))$, the area of the red trapezoid.

error terms

For the polynomial p interpolating f at points x_0, x_1, ..., x_n, we have

$$p(x) = f(x) + \frac{f^{n+1}(\alpha)}{(n+1)!}(x - x_0)(x - x_1)\cdots(x - x_n),$$

for some $\alpha \in [a, b]$.

Then we can derive the following error formula:

$$\int_a^b f(x)dx = \int_a^b p(x)dx - \frac{f^{n+1}(\alpha)}{(n+1)!}\int_a^b (x - x_0)(x - x_1)\cdots(x - x_n)dx.$$

So we have the error is

$$\left| \frac{f^{n+1}(\alpha)}{(n+1)!}\int_a^b (x - x_0)(x - x_1)\cdots(x - x_n)dx \right|.$$

the error of the trapezoidal rule

$$\int_a^b f(x)dx \approx \frac{b-a}{2}\left(f(a)+f(b)\right).$$

We have $x_0 = a$ and $x_1 = b$ in the error formula:

$$\left| \frac{f^{n+1}(\alpha)}{(n+1)!} \int_a^b (x-x_0)(x-x_1)\cdots(x-x_n)dx \right|.$$

We compute:

$$\int_a^b (x-a)(x-b)dx = \frac{(b-a)^3}{6}.$$

So the error for the trapezoidal rule is $\left| \frac{f''(\alpha)}{12} \right| (b-a)^3$.

Exercise 1:

Compute the error formula for the midpoint rule.

degree of precision

The cost of a quadrature rule is determined by the number of function values, or equivalently, the number of interpolation points.

Definition

A quadrature rule has *degree of precision* d
if the rule integrates all polynomials of degree d or less exactly.

Because $\int_a^b$ is a linear operator:

$$\int_a^b c_d x^d + \cdots + c_1 x + c_0 dx = \int_a^b c_d x^d dx + \cdots + \int_a^b c_1 x dx + \int_a^b c_0 dx,$$

it suffices to compute the degree of precision for the basis functions.

the degree of precision of the midpoint rule

$$\int_a^b f(x)dx \approx R(f), \quad R(f) = (b-a)f\left(\frac{a+b}{2}\right).$$

$$f = 1 \quad : \quad \int_a^b 1dx = b - a, \quad R(1) = b - a$$

$$f = x \quad : \quad \int_a^b xdx = \frac{b^2}{2} - \frac{a^2}{2}, \quad R(x) = (b-a)(a+b)/2$$

$$f = x^2 \quad : \quad \int_a^b x^2dx = \frac{b^3}{3} - \frac{a^3}{3}, \quad R(x^2) = (b-a)((a+b)/2)^2$$

We see that $R(1)$ and $R(x)$ are exact, but $R(x^2) \neq \displaystyle\int_a^b x^2dx$.

Exercise 2:
Compute the degree of precision of the trapezoidal rule.

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deriving a quadrature rule

Determine the weights w_0, w_1 and w_2 in

$$\int_a^b f(x)dx \approx w_0 f(a) + w_1 f\left(\frac{a+b}{2}\right) + w_2 f(b),$$

so the degree of precision is as high as possible.

$$\begin{aligned}
f = 1 \quad &: \quad \int_a^b 1dx = b - a = w_0 + w_1 + w_2 \\
f = x \quad &: \quad \int_a^b xdx = \frac{b^2}{2} - \frac{a^2}{2} = w_0 a + w_1 \left(\frac{a+b}{2}\right) + w_2 b \\
f = x^2 \quad &: \quad \int_a^b x^2 dx = \frac{b^3}{3} - \frac{a^3}{3} = w_0 a^2 + w_1 \left(\frac{a+b}{2}\right)^2 + w_2 b^2
\end{aligned}$$

solving a linear system

$$\begin{aligned}
\int_a^b 1 dx = b - a &= w_0 + w_1 + w_2 \\
\int_a^b x dx = \frac{b^2}{2} - \frac{a^2}{2} &= w_0 a + w_1 \left(\frac{a+b}{2} \right) + w_2 b \\
\int_a^b x^2 dx = \frac{b^3}{3} - \frac{a^3}{3} &= w_0 a^2 + w_1 \left(\frac{a+b}{2} \right)^2 + w_2 b^2
\end{aligned}$$

In matrix format:

$$\begin{bmatrix} 1 & a & a^2 \\ 1 & (a+b)/2 & ((a+b)/2)^2 \\ 1 & b & b^2 \end{bmatrix} \begin{bmatrix} w_0 \\ w_1 \\ w_2 \end{bmatrix} = \begin{bmatrix} b - a \\ b^2/2 - a^2/2 \\ b^3/3 - a^3/3 \end{bmatrix}$$

Observe the structure: we have a Vandermonde matrix.

solving with SymPy gives Simpson's rule

```
julia> using SymPy
julia> a,b,w0,w1,w2 = Sym("a,b,w0,w1,w2");
julia> eq1 = w0 + w1 + w2;
julia> eq2 = a*w0 + (a+b)*w1/2 + b*w2;
julia> eq3 = a^2*w0 + (a+b)^2*w1/4 + b^2*w2;
julia> solve([eq1 - b+a,
              eq2 - b^2/2 + a^2/2,
              eq3 - b^3/3 + a^3/3], [w0,w1,w2])
Dict{Any,Any} with 3 entries:
  w2 => -a/6 + b/6
  w0 => -a/6 + b/6
  w1 => -2*a/3 + 2*b/3
```

$$\int_a^b f(x)dx \approx \left(\frac{b-a}{6}\right) f(a) + 2\left(\frac{b-a}{3}\right) f\left(\frac{a+b}{2}\right) + \left(\frac{b-a}{6}\right) f(b)$$

making another quadrature rule

Exercise 3:

Consider the quadrature rule

$$\int_{-a}^{a} f(x)dx \approx w_1 f\left(\frac{-a}{2}\right) + w_2 f\left(\frac{a}{2}\right), \quad \text{for} \quad a > 0.$$

1. Determine the weights w_1 and w_2 to obtain the highest possible degree of precision.
2. What is the degree of precision of your rule? Verify for 1, x, and also x^2.

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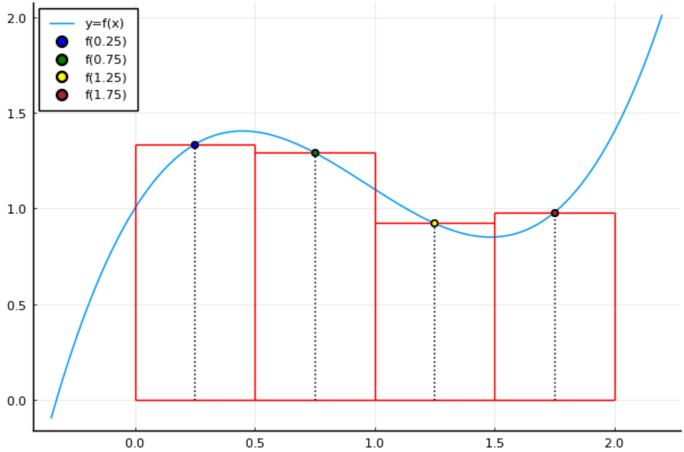
the composite midpoint rule



$\displaystyle\int_0^2 f(x)dx$, the area under the blue curve, for $x \in [0, 2]$,

is approximated by the sum of the areas of four red rectangles.

composite quadrature rules

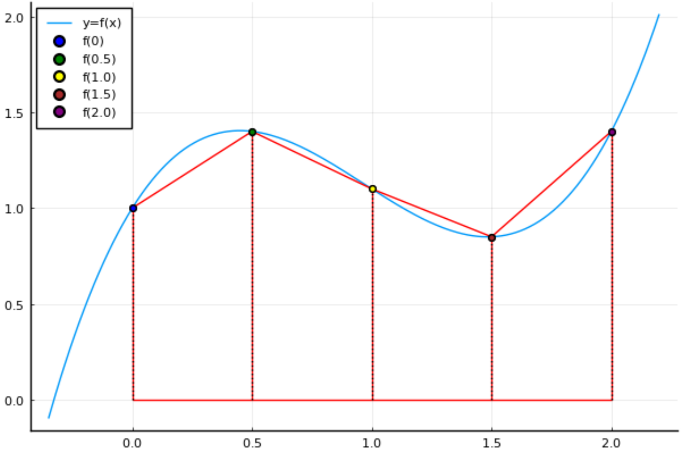
A composite quadrature rule over $[a, b]$ consists in

1. dividing $[a, b]$ in n subintervals, $h = (b - a)/n$;
2. applying a quadrature rule to each subinterval $[a_i, b_i]$, with $a_i = a + (i - 1)h$, and $b_i = a + ih$, for $i = 1, 2, \ldots, n$;
3. summing up the approximations on each subinterval.

Example: $[a, b] = [0, 1]$, $n = 4$: $h = 1/4$, and
the subintervals are $[0, 1/4]$, $[1/4, 1/2]$, $[1/2, 3/4]$, $[3/4, 1]$.

Exercise 4:
Derive the formula for the composite midpoint rule over n subintervals to approximate the integral of $f(x)$ over $[a, b]$.

the composite trapezoidal rule



$\int_0^2 f(x)dx$, the area under the blue curve, for $x \in [0, 2]$,

is approximated by the sum of the areas of four red trapezoids.

the composite trapezoidal rule

For $n = 1$:

$$\int_a^b f(x)dx \approx \frac{b-a}{2}\left(f(a) + f(b)\right).$$

For $n > 1$, $h = (b-a)/n$, $a_i = a + (i-1)h$, $b_i = a + ih$:

$$\begin{aligned}\int_a^b f(x)dx &= \sum_{i=1}^{n} \int_{a_i}^{b_i} f(x)dx \\ &= \sum_{i=1}^{n} \frac{h}{2}\Big(f(a_i) + f(b_i)\Big) \\ &= \frac{h}{2}\Big(f(a) + f(b)\Big) + h\sum_{i=1}^{n-1} f(a+ih)\end{aligned}$$

Observe that $a_i = b_{i-1}$ and the value $f(b_{i-1})$ at the right of the $(i-1)$-th interval equals the value $f(a_i)$ at the left of the i-th interval.

the error of the composite trapezoidal rule

The error of the trapezoidal rule for f over $[a,b]$ is

$$\left| \frac{f''(\alpha)}{12} \right| (b-a)^3,$$

for some $\alpha \in [a,b]$. For the composite rule over n subintervals, the length of each subinterval is $h = (b-a)/n$.
The error of the composite trapezoidal rule is then

$$\sum_{i=1}^{n} \left| \frac{f''(\alpha_i)}{12} \right| h^3,$$

for $\alpha_i \in [a_i, b_i]$. If we apply the mean value theorem on f'', then there exists an $\alpha \in [a,b]$ such that $nf''(\alpha)$ is the sum over all $f''(\alpha_i)$'s.
The error is then $\left| \frac{nf''(\alpha)}{12} \right| h^3 = \left(\frac{b-a}{12} \right) |f''(\alpha)| h^2$, which is $O(h^2)$.

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a Julia function

```
"""
Applies the composite trapezoidal rule to approximate
the integral of the function f over the interval [a,b],
using n subintervals.

Example: t = comptrap(cos,0,pi/2,100)
"""
function comptrap(f::Function,a::Float64,
                  b::Float64,n::Int64)
    h = (b-a)/n
    t = (f(a) + f(b))/2
    for i = 1:n-1
        t = t + f(a+i*h)
    end
    t = t*h
    return t
end
```

testing the `comptrap` function

```
"""
Applies the composite trapezoidal rule
to the area under the unit circle.
"""
function main()
   f(x) = sqrt(1 - x^2)
   exact = pi/4
   N = 1
   for i=1:21
       t = comptrap(f,0.0,1.0,N)
       strnbr = @sprintf("%7d", N)
       strval = @sprintf("%.16e", t)
       strerr = @sprintf("%.2e", abs(t-exact))
       println(" $strnbr  $strval  $strerr")
       N = 2*N
   end
end
```

running the program

```
      1   5.000000000000000e-01   2.85e-01
      2   6.830127018922193e-01   1.02e-01
      4   7.489272670256101e-01   3.65e-02
      8   7.724547860892933e-01   1.29e-02
     16   7.808132594569353e-01   4.58e-03
     32   7.837756057192827e-01   1.62e-03
     64   7.848242281949214e-01   5.74e-04
    128   7.851951980991536e-01   2.03e-04
    256   7.853263957393075e-01   7.18e-05
    512   7.853727881799136e-01   2.54e-05
   1024   7.853891916347549e-01   8.97e-06
   2048   7.853949913528606e-01   3.17e-06
   4096   7.853970419019397e-01   1.12e-06
   8192   7.853977668874225e-01   3.97e-07
  16384   7.853980232097232e-01   1.40e-07
  32768   7.853981138335608e-01   4.96e-08
  65536   7.853981458739598e-01   1.75e-08
 131072   7.853981572019569e-01   6.20e-09
 262144   7.853981612070172e-01   2.19e-09
 524288   7.853981626230216e-01   7.74e-10
1048576   7.853981631236601e-01   2.74e-10
```

cost and convergence

Doubling the number of function evaluations,

```
  524288  7.853981626230216 5e-01  7.74e-10
 1048576  7.853981631236601 8e-01  2.74e-10
```

from 524,288 to 1,048,576, the error decreases from 7.7×10^{-10} to 2.7×10^{-10}, a reduction factor of 2.85.

The convergence is linear, and too slow.

Exercise 5:

Apply the composite midpoint rule to $\displaystyle\int_0^1 \sqrt{1 - x^2} dx$

for a number of intervals ranging from 1 to 2^{20}.

Describe the convergence? Compare with the application of the composite trapezoidal rule to this problem.

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Newton-Cotes Formulas

To approximate $\int_a^b f(x)dx$, with $n+1$ function evaluations:

1. Let $h = (b-a)/n$ and set $x_i = a + i\,h$, for $i = 0, 1, \ldots, n$.
2. Let p be the polynomial interpolating at $(x_i, f(x_i))$: $p(x_i) = f(x_i)$.
3. Then the rule is

$$\int_a^b p(x)dx \quad \text{with error term} \quad E = \left| \int_a^b \prod_{i=0}^{n} (x - x_i) dx \right| .$$

Such rules are called *Newton-Cotes formulas*.

We have seen two examples:

1. $n = 1$: the trapezoidal rule,
2. $n = 2$: Simpson's rule.

recall Lagrange interpolation

Given (x_i, f_i), for $i = 0, 1, \ldots, n$, and for any $j \neq i$: $x_j \neq x_i$, the Lagrange form of the interpolating polynomial p is

$$p(x) = f_0\ell_0(x) + f_1\ell_1(x) + \cdots + f_n\ell_n(x), \quad \ell_i(x) = \prod_{\substack{j=0 \\ j \neq i}}^{n} \left(\frac{x - x_j}{x_i - x_j} \right).$$

Then the quadrature rule is

$$\int_a^b p(x)dx = f_0 \underbrace{\int_a^b \ell_0(x)dx}_{w_0} + f_1 \underbrace{\int_a^b \ell_1(x)dx}_{w_1} + \cdots + f_n \underbrace{\int_a^b \ell_n(x)dx}_{w_n}.$$

The weights of the Newton-Cotes formulas are the integrals of the Lagrange polynomials.